

tert-Butylhydroquinone
1948-33-0 | DTXSID6020220

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 18.8

Global applicability domain: Inside

Local applicability domain index: 4.75e-01

Confidence level: 6.60e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>O,O-Diethyl dithiophosphate</div> <div>Measured: 5.01</div> <div>Predicted: 5.43</div>	<div>Image not found</div> <div>Methyl parathion</div> <div>Measured: 85.1</div> <div>Predicted: 14.5</div>	<div>Image not found</div> <div>Dioxabenzofos</div> <div>Measured: 20.4</div> <div>Predicted: 13.7</div>
<div>Image not found</div> <div>Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>	<div>Image not found</div> <div>(1R,2S,5R)-(-)-Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>	<div>Image not found</div> <div>Cyanophos</div> <div>Measured: 36.3</div> <div>Predicted: 7.14</div>